



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:58 pm GMT

PDB ID : 3DOR
Title : Crystal Structure of mature CPAF
Authors : Chai, J.; Huang, Z.
Deposited on : 2008-07-06
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

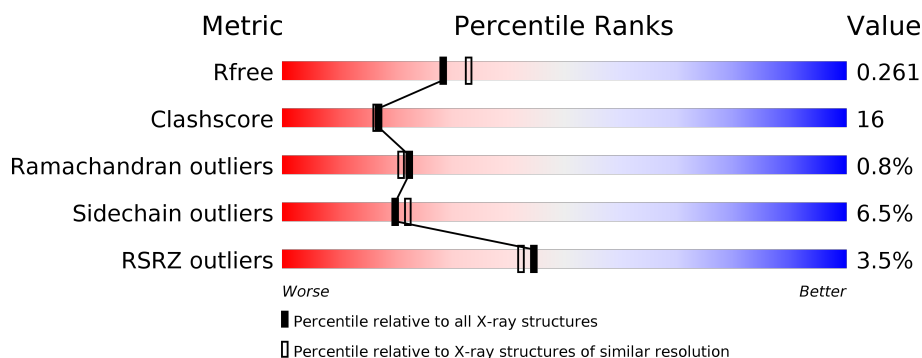
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	583	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>29%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	583	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>21%</div> <div>•</div> <div>10%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8746 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein CT_858.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4105	2627	688	777	13			
1	B	527	Total	C	N	O	S	0	0	0
			4141	2652	693	783	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	610	HIS	-	EXPRESSION TAG	UNP O84866
A	611	HIS	-	EXPRESSION TAG	UNP O84866
A	612	HIS	-	EXPRESSION TAG	UNP O84866
A	613	HIS	-	EXPRESSION TAG	UNP O84866
A	614	HIS	-	EXPRESSION TAG	UNP O84866
A	615	HIS	-	EXPRESSION TAG	UNP O84866
B	610	HIS	-	EXPRESSION TAG	UNP O84866
B	611	HIS	-	EXPRESSION TAG	UNP O84866
B	612	HIS	-	EXPRESSION TAG	UNP O84866
B	613	HIS	-	EXPRESSION TAG	UNP O84866
B	614	HIS	-	EXPRESSION TAG	UNP O84866
B	615	HIS	-	EXPRESSION TAG	UNP O84866

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

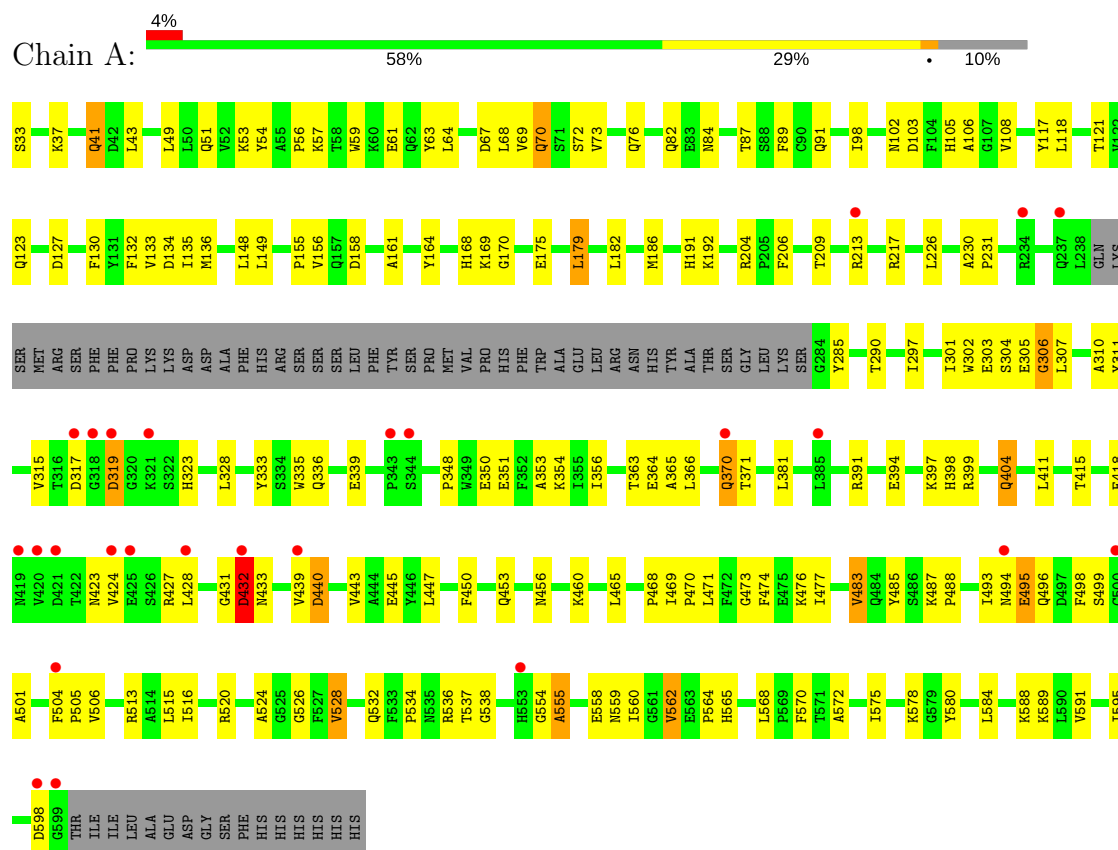
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	140	Total	O	0	0
			140	140		
3	B	285	Total	O	0	0
			285	285		

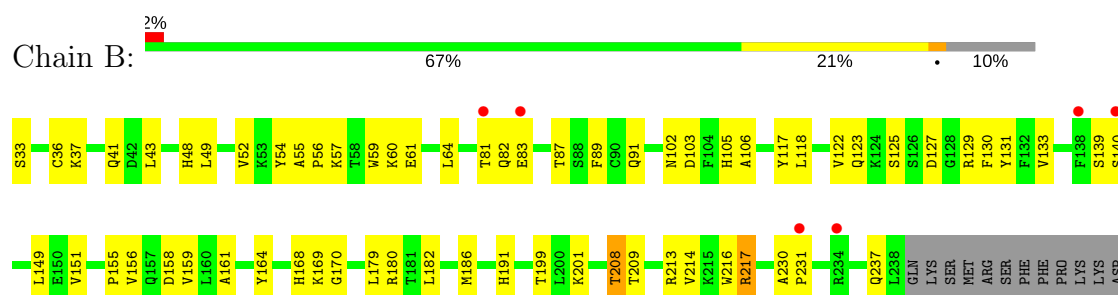
3 Residue-property plots [i](#)

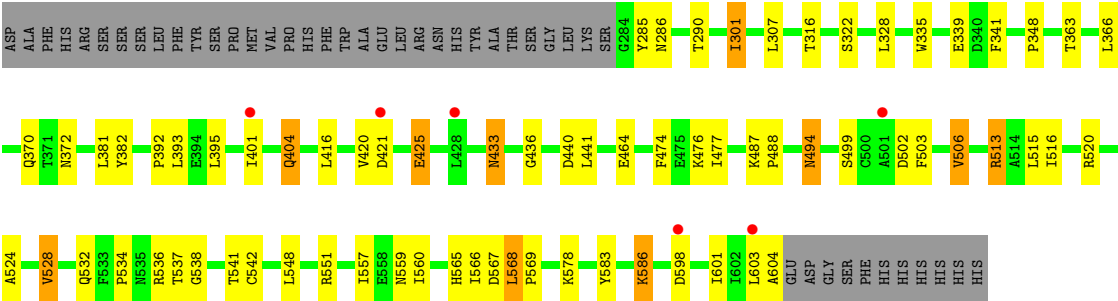
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein CT_858



• Molecule 1: Protein CT_858





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.30Å 152.37Å 162.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.27 – 2.20 39.27 – 2.19	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.27-2.20) 99.0 (39.27-2.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.262 0.226 , 0.261	Depositor DCC
R_{free} test set	3937 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8746	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/4203	0.62	0/5713
1	B	0.38	0/4239	0.65	0/5763
All	All	0.37	0/8442	0.64	0/11476

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4105	0	4043	154	0
1	B	4141	0	4088	121	0
2	A	45	0	0	1	0
2	B	30	0	0	1	0
3	A	140	0	0	2	0
3	B	285	0	0	4	0
All	All	8746	0	8131	257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:LYS:HE2	1:B:603:LEU:HD23	1.40	0.99
1:B:59:TRP:HE1	1:B:559:ASN:HD22	1.07	0.98
1:A:59:TRP:HE1	1:A:559:ASN:HD22	1.10	0.95
1:A:494:ASN:HD22	1:A:496:GLN:H	0.92	0.91
1:A:494:ASN:HD22	1:A:496:GLN:N	1.65	0.91
1:B:516:ILE:H	1:B:565:HIS:HD2	1.17	0.91
1:B:586:LYS:CE	1:B:603:LEU:HD23	2.03	0.88
1:A:516:ILE:H	1:A:565:HIS:HD2	1.21	0.87
1:A:297:ILE:HB	1:A:588:LYS:HD3	1.57	0.85
1:A:432:ASP:HA	1:A:439:VAL:HB	1.57	0.84
1:A:335:TRP:HB2	1:A:348:PRO:HG3	1.60	0.84
1:B:54:TYR:CZ	1:B:56:PRO:HG2	2.14	0.82
1:A:570:PHE:HB3	1:A:575:ILE:HD11	1.61	0.81
1:A:534:PRO:HG2	1:B:49:LEU:HD22	1.62	0.80
1:A:570:PHE:HB3	1:A:575:ILE:CD1	2.12	0.79
1:B:586:LYS:CE	1:B:604:ALA:H	1.96	0.77
1:A:33:SER:O	1:A:37:LYS:HG3	1.85	0.76
1:A:427:ARG:HB3	1:A:432:ASP:HB3	1.68	0.74
1:A:133:VAL:O	1:A:578:LYS:HD3	1.88	0.73
1:A:516:ILE:H	1:A:565:HIS:CD2	2.05	0.73
1:B:82:GLN:HG3	1:B:89:PHE:CE2	2.23	0.73
1:A:538:GLY:HA2	1:B:404:GLN:CG	2.20	0.72
1:A:57:LYS:O	1:A:61:GLU:HG3	1.89	0.72
1:A:186:MET:H	1:A:191:HIS:HD2	1.39	0.70
1:A:494:ASN:ND2	1:A:496:GLN:H	1.77	0.69
1:A:404:GLN:CG	1:B:538:GLY:HA2	2.22	0.69
1:A:49:LEU:HD22	1:B:534:PRO:HG2	1.74	0.68
1:A:487:LYS:HB3	1:A:488:PRO:HD2	1.74	0.68
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.59	0.68
1:A:54:TYR:CZ	1:A:56:PRO:HG2	2.29	0.67
1:A:105:HIS:CE1	1:A:528:VAL:HG22	2.30	0.66
1:B:105:HIS:CG	1:B:528:VAL:HG13	2.31	0.66
1:A:121:THR:HB	1:A:134:ASP:HB3	1.78	0.66
1:B:316:THR:HG22	1:B:322:SER:OG	1.96	0.65
1:B:123:GLN:HE21	1:B:133:VAL:HG11	1.62	0.64
1:B:516:ILE:H	1:B:565:HIS:CD2	2.07	0.64
1:B:395:LEU:HD21	1:B:477:ILE:HD12	1.79	0.64
1:B:586:LYS:NZ	1:B:603:LEU:HD23	2.13	0.63
1:A:64:LEU:HD23	1:A:169:LYS:HD2	1.79	0.63
1:A:186:MET:H	1:A:191:HIS:CD2	2.16	0.63
1:A:424:VAL:HA	1:A:427:ARG:NH1	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:GLY:HA2	1:B:404:GLN:HG3	1.81	0.63
1:A:404:GLN:H	1:A:404:GLN:NE2	1.97	0.62
1:B:54:TYR:CE2	1:B:56:PRO:HG2	2.35	0.62
1:A:161:ALA:HA	1:A:164:TYR:CD2	2.33	0.62
1:A:315:VAL:HG12	1:A:323:HIS:HB2	1.81	0.62
1:A:404:GLN:HG3	1:B:538:GLY:HA2	1.80	0.62
1:A:353:ALA:HB1	1:A:483:VAL:HG11	1.82	0.62
1:A:424:VAL:O	1:A:428:LEU:HD13	2.00	0.61
1:B:87:THR:O	1:B:91:GLN:HG3	2.01	0.61
1:B:186:MET:H	1:B:191:HIS:CD2	2.19	0.60
1:B:404:GLN:NE2	1:B:404:GLN:H	1.99	0.60
1:B:64:LEU:HD23	1:B:169:LYS:HD2	1.84	0.60
1:B:59:TRP:HE1	1:B:559:ASN:ND2	1.88	0.59
1:A:63:TYR:CD2	1:A:64:LEU:HG	2.37	0.59
1:B:81:THR:O	1:B:81:THR:HG22	2.02	0.59
1:A:51:GLN:HG3	1:A:68:LEU:CD2	2.33	0.59
1:A:440:ASP:H	1:A:443:VAL:CG2	2.16	0.59
1:A:506:VAL:HG23	1:A:562:VAL:CG2	2.33	0.59
1:A:394:GLU:OE2	1:A:476:LYS:HE2	2.03	0.58
1:B:395:LEU:HD21	1:B:477:ILE:CD1	2.33	0.58
1:B:290:THR:OG1	1:B:339:GLU:HB2	2.03	0.58
1:B:416:LEU:O	1:B:416:LEU:HD23	2.04	0.58
1:B:149:LEU:O	1:B:156:VAL:HG23	2.03	0.58
1:B:151:VAL:HB	1:B:159:VAL:HG21	1.85	0.57
1:B:586:LYS:HE3	3:B:860:HOH:O	2.04	0.57
1:B:33:SER:N	1:B:37:LYS:HZ3	2.02	0.57
1:A:538:GLY:CA	1:B:404:GLN:HG3	2.34	0.57
1:A:63:TYR:HD2	1:A:64:LEU:HG	1.67	0.57
1:A:432:ASP:CA	1:A:439:VAL:HB	2.32	0.57
1:B:33:SER:N	1:B:37:LYS:NZ	2.52	0.56
1:A:584:LEU:O	1:A:588:LYS:HG3	2.05	0.56
1:A:411:LEU:O	1:A:415:THR:HG23	2.05	0.56
1:A:554:GLY:O	1:A:555:ALA:HB3	2.06	0.56
1:B:201:LYS:HE3	1:B:209:THR:HG21	1.87	0.56
1:A:290:THR:OG1	1:A:339:GLU:HB2	2.05	0.56
1:B:401:ILE:HG12	1:B:464:GLU:O	2.05	0.56
1:A:310:ALA:HB2	1:A:328:LEU:HD23	1.88	0.55
1:A:397:LYS:HB2	1:A:468:PRO:HB2	1.88	0.55
1:B:372:ASN:H	1:B:494:ASN:HD21	1.54	0.55
1:A:456:ASN:OD1	1:A:460:LYS:HE3	2.07	0.55
1:A:506:VAL:HG23	1:A:562:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:GLN:HG3	1:B:538:GLY:CA	2.37	0.55
1:B:186:MET:H	1:B:191:HIS:HD2	1.52	0.54
1:A:538:GLY:HA2	1:B:404:GLN:HG2	1.89	0.54
1:A:536:ARG:HA	1:B:404:GLN:HE22	1.73	0.54
1:A:589:LYS:HB2	1:A:589:LYS:NZ	2.23	0.54
1:A:336:GLN:CD	1:A:336:GLN:H	2.10	0.53
1:A:399:ARG:HH21	1:A:465:LEU:HD23	1.73	0.53
1:A:494:ASN:ND2	1:A:496:GLN:N	2.46	0.53
1:B:301:ILE:HD12	1:B:301:ILE:O	2.08	0.53
1:B:586:LYS:HZ1	1:B:603:LEU:HD23	1.73	0.53
1:B:55:ALA:HA	1:B:401:ILE:HG13	1.89	0.53
1:B:55:ALA:CA	1:B:401:ILE:HG13	2.38	0.53
1:B:420:VAL:HG13	1:B:425:GLU:HB3	1.89	0.53
1:A:504:PHE:HB3	1:A:505:PRO:CD	2.39	0.53
1:A:570:PHE:CB	1:A:575:ILE:HD11	2.36	0.53
1:B:603:LEU:O	1:B:604:ALA:HB2	2.08	0.53
1:A:536:ARG:HA	1:B:404:GLN:NE2	2.24	0.53
1:A:365:ALA:HB2	1:A:595:ILE:HD11	1.91	0.53
1:B:328:LEU:C	1:B:328:LEU:HD13	2.29	0.53
1:B:603:LEU:O	1:B:604:ALA:CB	2.57	0.53
1:A:297:ILE:HB	1:A:588:LYS:CD	2.35	0.52
1:A:67:ASP:HB3	1:A:70:GLN:HB2	1.90	0.52
1:B:103:ASP:HB3	1:B:106:ALA:HB3	1.90	0.52
1:B:125:SER:OG	1:B:127:ASP:OD2	2.27	0.52
1:A:41:GLN:HG3	1:B:48:HIS:CD2	2.44	0.52
1:A:123:GLN:HE21	1:A:133:VAL:HG11	1.75	0.52
1:A:371:THR:HG22	1:A:494:ASN:HB2	1.92	0.52
1:A:499:SER:H	1:A:524:ALA:HB3	1.74	0.52
1:A:117:TYR:HD2	1:A:217:ARG:HD2	1.75	0.51
1:A:303:GLU:HA	1:A:311:TYR:HA	1.92	0.51
1:A:520:ARG:HD2	1:A:560:ILE:O	2.09	0.51
1:B:433:ASN:ND2	1:B:436:GLY:H	2.08	0.51
1:A:520:ARG:NH2	2:A:619:SO4:S	2.83	0.51
1:A:69:VAL:O	1:A:73:VAL:HG23	2.10	0.51
1:B:335:TRP:HB2	1:B:348:PRO:HG3	1.93	0.51
1:B:118:LEU:HD22	1:B:214:VAL:CG1	2.41	0.51
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.23	0.50
1:B:33:SER:HB3	1:B:36:CYS:HB3	1.94	0.50
1:A:415:THR:HA	1:A:418:GLU:HG3	1.92	0.50
1:A:105:HIS:CG	1:A:528:VAL:HG22	2.47	0.50
1:A:431:GLY:C	1:A:433:ASN:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HG	1:B:216:TRP:CE3	2.47	0.50
1:B:566:ILE:HG23	1:B:603:LEU:HD12	1.94	0.50
1:B:586:LYS:HE2	1:B:604:ALA:H	1.76	0.50
1:A:307:LEU:HB2	1:A:351:GLU:OE1	2.12	0.49
1:A:350:GLU:O	1:A:354:LYS:HG2	2.12	0.49
1:A:105:HIS:ND1	1:A:528:VAL:HG22	2.27	0.49
1:B:568:LEU:HD13	1:B:583:TYR:CD1	2.47	0.49
1:B:586:LYS:HE2	1:B:603:LEU:CD2	2.28	0.49
1:A:516:ILE:N	1:A:565:HIS:HD2	2.01	0.49
1:A:365:ALA:CB	1:A:595:ILE:HD11	2.43	0.49
1:B:393:LEU:HD21	1:B:513:ARG:HG3	1.94	0.49
1:A:447:LEU:O	1:A:450:PHE:O	2.30	0.49
1:A:356:ILE:HG23	1:A:485:TYR:HB2	1.94	0.49
1:A:315:VAL:HG23	1:A:588:LYS:HB3	1.95	0.49
1:B:55:ALA:HB2	1:B:401:ILE:HG13	1.95	0.49
1:B:335:TRP:HB2	1:B:348:PRO:CG	2.43	0.48
1:B:537:THR:HG22	1:B:537:THR:O	2.13	0.48
1:B:499:SER:O	1:B:502:ASP:HB2	2.13	0.48
1:A:404:GLN:H	1:A:404:GLN:CD	2.14	0.48
1:A:87:THR:O	1:A:91:GLN:HG3	2.13	0.48
1:B:117:TYR:O	1:B:217:ARG:HB2	2.13	0.48
1:B:286:ASN:HB2	3:B:673:HOH:O	2.13	0.48
1:B:60:LYS:NZ	1:B:559:ASN:HD21	2.12	0.48
1:B:487:LYS:HB3	1:B:488:PRO:HD2	1.96	0.47
1:B:55:ALA:HA	1:B:401:ILE:CG1	2.44	0.47
1:B:601:ILE:N	1:B:601:ILE:HD12	2.29	0.47
1:A:591:VAL:O	1:A:595:ILE:HD12	2.14	0.47
1:A:82:GLN:HG3	1:A:89:PHE:CE2	2.49	0.47
1:B:499:SER:H	1:B:524:ALA:HB3	1.79	0.47
1:B:155:PRO:HG2	1:B:158:ASP:OD2	2.14	0.47
1:B:341:PHE:CE1	1:B:348:PRO:HD3	2.50	0.47
1:A:371:THR:CG2	1:A:494:ASN:HB2	2.45	0.47
1:B:381:LEU:C	1:B:381:LEU:HD13	2.35	0.47
1:A:134:ASP:OD2	1:A:136:MET:SD	2.73	0.47
1:A:230:ALA:N	1:A:231:PRO:HD2	2.30	0.47
1:A:423:ASN:O	1:A:427:ARG:HG3	2.15	0.47
1:A:536:ARG:HG3	1:B:52:VAL:HG13	1.96	0.46
1:B:433:ASN:HD22	1:B:436:GLY:H	1.64	0.46
1:B:586:LYS:NZ	1:B:604:ALA:H	2.13	0.46
1:B:180:ARG:NE	2:B:617:SO4:O4	2.48	0.46
1:B:118:LEU:HD22	1:B:214:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:HIS:CE1	1:A:526:GLY:O	2.69	0.46
1:B:516:ILE:N	1:B:516:ILE:HD12	2.31	0.46
1:A:54:TYR:CE2	1:A:56:PRO:HG2	2.50	0.46
1:A:575:ILE:N	1:A:575:ILE:HD12	2.29	0.46
1:A:319:ASP:N	1:A:319:ASP:OD2	2.49	0.46
1:A:470:PRO:HB2	1:A:474:PHE:O	2.16	0.46
1:B:129:ARG:CZ	1:B:131:TYR:OH	2.64	0.46
1:B:392:PRO:HB2	1:B:476:LYS:HD3	1.97	0.46
1:B:122:VAL:HG11	1:B:130:PHE:HB3	1.98	0.46
1:A:130:PHE:HE2	1:A:179:LEU:HD21	1.81	0.45
1:A:53:LYS:HG3	1:B:534:PRO:CB	2.46	0.45
1:A:404:GLN:HE22	1:B:536:ARG:HA	1.82	0.45
1:A:558:GLU:O	1:A:559:ASN:HB2	2.15	0.45
3:A:739:HOH:O	1:B:404:GLN:HG2	2.16	0.45
1:A:371:THR:HB	1:A:494:ASN:HB2	1.99	0.45
1:A:333:TYR:CE2	1:A:381:LEU:HD23	2.51	0.45
1:A:404:GLN:HG2	1:B:538:GLY:HA2	1.96	0.45
1:A:161:ALA:HA	1:A:164:TYR:CE2	2.52	0.45
1:A:591:VAL:O	1:A:595:ILE:CD1	2.66	0.45
1:A:53:LYS:HG3	1:B:534:PRO:HB2	1.99	0.45
1:A:431:GLY:O	1:A:432:ASP:CG	2.55	0.44
1:A:43:LEU:C	1:A:43:LEU:HD13	2.38	0.44
1:B:103:ASP:OD1	1:B:105:HIS:HB2	2.17	0.44
1:B:57:LYS:O	1:B:61:GLU:HG3	2.18	0.44
1:A:149:LEU:O	1:A:156:VAL:HG23	2.16	0.44
1:A:494:ASN:ND2	1:A:495:GLU:N	2.65	0.44
1:A:440:ASP:H	1:A:443:VAL:HG23	1.82	0.44
1:A:285:TYR:CE1	1:A:578:LYS:HD2	2.53	0.44
1:B:161:ALA:HA	1:B:164:TYR:CD2	2.53	0.44
1:B:381:LEU:HD12	1:B:382:TYR:CD1	2.53	0.44
1:B:201:LYS:CE	1:B:209:THR:HG21	2.48	0.44
1:A:204:ARG:NH2	3:A:647:HOH:O	2.48	0.44
1:B:536:ARG:HG3	1:B:536:ARG:HH11	1.81	0.44
1:A:168:HIS:CE1	1:A:170:GLY:HA2	2.51	0.44
1:A:450:PHE:HB2	1:A:473:GLY:CA	2.48	0.44
1:A:493:ILE:HD11	1:A:564:PRO:HB3	2.00	0.44
1:B:105:HIS:CG	1:B:528:VAL:CG1	3.01	0.44
1:B:503:PHE:O	1:B:506:VAL:HG12	2.17	0.44
1:A:506:VAL:HG23	1:A:562:VAL:HG22	1.98	0.43
1:B:55:ALA:CB	1:B:401:ILE:HG13	2.49	0.43
1:A:130:PHE:CE2	1:A:179:LEU:HD21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:TRP:HB2	1:A:348:PRO:CG	2.40	0.43
1:B:566:ILE:CG2	1:B:603:LEU:HD12	2.48	0.43
1:B:168:HIS:CE1	1:B:170:GLY:HA2	2.54	0.43
1:A:495:GLU:H	1:A:495:GLU:CD	2.21	0.43
1:B:520:ARG:HD3	1:B:560:ILE:O	2.19	0.43
1:A:328:LEU:C	1:A:328:LEU:HD13	2.38	0.43
1:A:504:PHE:HB3	1:A:505:PRO:HD3	2.00	0.43
1:A:285:TYR:HE2	1:A:580:TYR:HH	1.67	0.43
1:A:537:THR:HG22	1:A:537:THR:O	2.18	0.43
1:B:551:ARG:HD2	1:B:557:ILE:CD1	2.49	0.43
1:A:98:ILE:HG13	1:A:108:VAL:CG2	2.49	0.42
1:A:301:ILE:C	1:A:301:ILE:HD12	2.38	0.42
1:A:575:ILE:CD1	1:A:575:ILE:N	2.82	0.42
1:B:208:THR:HB	3:B:748:HOH:O	2.20	0.42
1:A:134:ASP:C	1:A:135:ILE:HD12	2.39	0.42
1:B:474:PHE:N	1:B:474:PHE:CD1	2.87	0.42
1:B:586:LYS:HD3	1:B:586:LYS:HA	1.62	0.42
1:A:132:PHE:HB3	1:A:135:ILE:HD11	2.01	0.42
1:A:304:SER:O	1:A:306:GLY:N	2.52	0.42
1:A:285:TYR:HE1	1:A:578:LYS:HD2	1.85	0.42
1:B:285:TYR:OH	1:B:578:LYS:HG2	2.20	0.42
1:A:424:VAL:HA	1:A:427:ARG:HH12	1.84	0.42
1:A:155:PRO:HG2	1:A:158:ASP:OD2	2.19	0.42
1:A:301:ILE:HD12	1:A:302:TRP:HB2	2.02	0.42
1:A:427:ARG:HD3	1:A:432:ASP:HB2	2.02	0.42
1:A:470:PRO:HG2	1:A:473:GLY:HA2	2.02	0.42
1:B:551:ARG:CG	1:B:557:ILE:HD11	2.50	0.42
1:A:371:THR:CB	1:A:494:ASN:HB2	2.50	0.42
1:B:56:PRO:HB3	1:B:548:LEU:HD21	2.01	0.41
1:A:148:LEU:HG	1:A:156:VAL:CG2	2.50	0.41
1:A:217:ARG:NH1	1:A:217:ARG:CG	2.84	0.41
1:A:127:ASP:OD1	1:A:572:ALA:HB2	2.20	0.41
1:B:56:PRO:O	1:B:60:LYS:HG2	2.19	0.41
1:A:398:HIS:CD2	1:A:471:LEU:HG	2.55	0.41
1:A:498:PHE:N	1:A:501:ALA:HB3	2.35	0.41
1:A:453:GLN:HB3	1:A:469:ILE:HD12	2.03	0.41
1:A:570:PHE:HB3	1:A:575:ILE:HD13	1.95	0.41
1:A:72:SER:O	1:A:76:GLN:HG3	2.21	0.41
1:B:199:THR:OG1	1:B:213:ARG:HD3	2.21	0.41
1:B:105:HIS:ND1	1:B:528:VAL:HG13	2.35	0.41
1:A:103:ASP:HB3	1:A:106:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:HIS:HE1	3:B:650:HOH:O	2.04	0.41
1:B:55:ALA:HA	1:B:401:ILE:HD11	2.02	0.41
1:A:483:VAL:O	1:A:483:VAL:CG2	2.68	0.41
1:A:51:GLN:HG3	1:A:68:LEU:HD21	2.02	0.41
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.94	0.40
1:B:541:THR:HG22	1:B:542:CYS:N	2.36	0.40
1:A:370:GLN:HE21	1:A:370:GLN:HB3	1.61	0.40
1:A:399:ARG:NH2	1:B:237:GLN:O	2.54	0.40
1:B:567:ASP:OD1	1:B:569:PRO:HD3	2.22	0.40
1:B:230:ALA:N	1:B:231:PRO:HD2	2.36	0.40
1:B:551:ARG:HD2	1:B:557:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/583 (89%)	487 (94%)	25 (5%)	6 (1%)	15	12
1	B	523/583 (90%)	504 (96%)	17 (3%)	2 (0%)	38	41
All	All	1041/1166 (89%)	991 (95%)	42 (4%)	8 (1%)	22	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	GLU
1	B	83	GLU
1	A	598	ASP
1	B	139	SER
1	A	317	ASP
1	A	306	GLY
1	A	555	ALA

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Mol	Chain	Res	Type
1	A	432	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	451/506 (89%)	420 (93%)	31 (7%)	18	19
1	B	455/506 (90%)	427 (94%)	28 (6%)	21	24
All	All	906/1012 (90%)	847 (94%)	59 (6%)	20	22

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	70	GLN
1	A	84	ASN
1	A	102	ASN
1	A	175	GLU
1	A	179	LEU
1	A	182	LEU
1	A	192	LYS
1	A	206	PHE
1	A	209	THR
1	A	213	ARG
1	A	226	LEU
1	A	319	ASP
1	A	363	THR
1	A	364	GLU
1	A	366	LEU
1	A	370	GLN
1	A	391	ARG
1	A	404	GLN
1	A	432	ASP
1	A	440	ASP
1	A	445	GLU

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Mol	Chain	Res	Type
1	A	477	ILE
1	A	483	VAL
1	A	495	GLU
1	A	513	ARG
1	A	515	LEU
1	A	528	VAL
1	A	532	GLN
1	A	562	VAL
1	A	568	LEU
1	B	41	GLN
1	B	43	LEU
1	B	102	ASN
1	B	140	SER
1	B	179	LEU
1	B	182	LEU
1	B	208	THR
1	B	217	ARG
1	B	301	ILE
1	B	307	LEU
1	B	363	THR
1	B	366	LEU
1	B	370	GLN
1	B	404	GLN
1	B	421	ASP
1	B	425	GLU
1	B	433	ASN
1	B	440	ASP
1	B	441	LEU
1	B	494	ASN
1	B	506	VAL
1	B	513	ARG
1	B	515	LEU
1	B	528	VAL
1	B	532	GLN
1	B	568	LEU
1	B	586	LYS
1	B	598	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN

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Mol	Chain	Res	Type
1	A	84	ASN
1	A	123	GLN
1	A	168	HIS
1	A	191	HIS
1	A	404	GLN
1	A	494	ASN
1	A	559	ASN
1	A	565	HIS
1	A	593	GLN
1	A	596	ASN
1	B	48	HIS
1	B	84	ASN
1	B	102	ASN
1	B	123	GLN
1	B	167	ASN
1	B	168	HIS
1	B	191	HIS
1	B	286	ASN
1	B	404	GLN
1	B	433	ASN
1	B	456	ASN
1	B	494	ASN
1	B	496	GLN
1	B	532	GLN
1	B	559	ASN
1	B	565	HIS
1	B	596	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	616	-	4,4,4	0.91	0	6,6,6	0.33	0
2	SO4	A	617	-	4,4,4	0.89	0	6,6,6	0.47	0
2	SO4	A	618	-	4,4,4	0.88	0	6,6,6	0.38	0
2	SO4	A	619	-	4,4,4	0.95	0	6,6,6	0.36	0
2	SO4	A	620	-	4,4,4	0.94	0	6,6,6	0.34	0
2	SO4	A	621	-	4,4,4	0.94	0	6,6,6	0.36	0
2	SO4	A	622	-	4,4,4	0.66	0	6,6,6	0.30	0
2	SO4	A	623	-	4,4,4	0.62	0	6,6,6	0.24	0
2	SO4	A	624	-	4,4,4	0.69	0	6,6,6	0.36	0
2	SO4	B	616	-	4,4,4	0.98	0	6,6,6	0.36	0
2	SO4	B	617	-	4,4,4	0.70	0	6,6,6	0.31	0
2	SO4	B	618	-	4,4,4	0.66	0	6,6,6	0.30	0
2	SO4	B	619	-	4,4,4	0.85	0	6,6,6	0.34	0
2	SO4	B	620	-	4,4,4	0.75	0	6,6,6	0.37	0
2	SO4	B	621	-	4,4,4	0.93	0	6,6,6	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	616	-	-	0/0/0/0	0/0/0/0
2	SO4	A	617	-	-	0/0/0/0	0/0/0/0
2	SO4	A	618	-	-	0/0/0/0	0/0/0/0
2	SO4	A	619	-	-	0/0/0/0	0/0/0/0
2	SO4	A	620	-	-	0/0/0/0	0/0/0/0
2	SO4	A	621	-	-	0/0/0/0	0/0/0/0
2	SO4	A	622	-	-	0/0/0/0	0/0/0/0
2	SO4	A	623	-	-	0/0/0/0	0/0/0/0
2	SO4	A	624	-	-	0/0/0/0	0/0/0/0
2	SO4	B	616	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	617	-	-	0/0/0/0	0/0/0/0
2	SO4	B	618	-	-	0/0/0/0	0/0/0/0
2	SO4	B	619	-	-	0/0/0/0	0/0/0/0
2	SO4	B	620	-	-	0/0/0/0	0/0/0/0
2	SO4	B	621	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	619	SO4	1	0
2	B	617	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	522/583 (89%)	0.18	25 (4%) 31 30	27, 43, 66, 87	0
1	B	527/583 (90%)	-0.15	12 (2%) 61 58	20, 32, 52, 71	0
All	All	1049/1166 (89%)	0.01	37 (3%) 44 42	20, 38, 62, 87	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	ASP	4.6
1	A	428	LEU	4.5
1	A	598	ASP	4.3
1	A	599	GLY	4.2
1	A	344	SER	4.1
1	A	420	VAL	4.0
1	A	321	LYS	3.8
1	A	318	GLY	3.7
1	B	231	PRO	3.7
1	B	81	THR	3.7
1	A	319	ASP	3.6
1	B	598	ASP	3.3
1	A	424	VAL	3.2
1	A	343	PRO	3.0
1	B	138	PHE	2.9
1	A	494	ASN	2.7
1	A	425	GLU	2.6
1	A	385	LEU	2.6
1	A	500	CYS	2.5
1	B	603	LEU	2.5
1	A	213	ARG	2.4
1	A	419	ASN	2.4
1	A	504	PHE	2.4
1	A	370	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	83	GLU	2.3
1	B	428	LEU	2.3
1	A	234	ARG	2.3
1	B	401	ILE	2.3
1	B	234	ARG	2.3
1	A	317	ASP	2.2
1	B	501	ALA	2.2
1	B	421	ASP	2.1
1	A	237	GLN	2.1
1	A	421	ASP	2.1
1	A	439	VAL	2.1
1	B	140	SER	2.1
1	A	553	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	B	616	5/5	0.95	0.22	0.39	61,61,62,63	0
2	SO4	B	619	5/5	0.99	0.11	0.04	37,40,41,42	0
2	SO4	A	617	5/5	0.98	0.11	-0.68	34,36,37,39	0
2	SO4	A	616	5/5	0.99	0.06	-4.31	35,35,37,38	0
2	SO4	A	621	5/5	0.94	0.27	-	75,75,75,76	0
2	SO4	A	622	5/5	0.92	0.23	-	69,70,70,70	0
2	SO4	A	618	5/5	0.94	0.14	-	56,57,58,59	0
2	SO4	B	620	5/5	0.96	0.18	-	60,61,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	618	5/5	0.92	0.34	-	72,72,73,75	0
2	SO4	A	620	5/5	0.82	0.32	-	76,76,77,78	0
2	SO4	A	624	5/5	0.90	0.47	-	70,71,71,72	0
2	SO4	A	623	5/5	0.91	0.48	-	77,77,77,79	0
2	SO4	B	621	5/5	0.95	0.20	-	62,63,64,64	0
2	SO4	A	619	5/5	0.90	0.18	-	71,71,71,71	0
2	SO4	B	617	5/5	0.99	0.07	-	46,49,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.